

Pseudo-gap behavior in dynamical properties of high- T_c cuprates

Tôru Sakai and Yoshinori Takahashi

Faculty of Science, Himeji Institute of Technology, Kamigori, Ako-gun, Hyogo 678-1297, Japan
(June 98)

Dynamical properties of 2D antiferromagnets with hole doping are investigated to see the effects of short range local magnetic order on the temperature dependence of the dynamical magnetic susceptibility. We show the pseudo-gap like behavior of the temperature dependence of the NMR relaxation rate. We also discuss implications of the results in relations to the observed spin gap like behavior of low-doped copper oxide high- T_c superconductors.

The spin-gap-like behavior observed in some low-doped high- T_c cuprates by dynamical measurements [1] have recently attracted much interest. The term “gap” originally arose because of the appearance of a broad peak above T_c in the temperature dependence of the NMR relaxation time measurements. It is, however, not clear whether the gaplike behavior is really associated with the opening of the energy gap in the excitation spectrum of the system, because the presence of superconductivity does not allow the measurement of the temperature-dependent properties at low temperature.

There have been several theoretical explanations for the origin of the gaplike behavior, for instance, a spinon singlet formation mechanism [2] and a CuO_2 bilayer coupling mechanism. [3,4] Its origin is, however, still controversial and is debatable. The purpose of the present paper is to propose a new theoretical explanation for the origin of the observed pseudogap behavior of cuprate superconductors.

Our idea is based on the observation that the pseudo-gap behavior is characteristic of low-doped cuprates, including, in particular, the pure undoped 2D Heisenberg antiferromagnets as an extreme case. We also assume that it is a property already present in the single-layer system, noting the fact that the gaplike behaviors are observed even in single-layer high- T_c cuprates. [5] It is then quite natural to assume that the observed pseudogap behavior will arise as a result of the short-range magnetic order (SRO) of the low-dimensional Heisenberg antiferromagnets with lowering of the temperature. The gaplike behavior has also been discussed in associating with the antiferromagnetic correlations in terms of the spin fluctuation theory. [6] Our purpose is to test this concept by explicit numerical diagonalization of the t - J model.

In low-dimensional magnets, even if there appears no long-range magnetic order, SRO begins to grow when the temperature of the system decreases below the characteristic temperature, which is of the same magnitude as the magnetic coupling constant. The excitation spectrum of the system is then affected by the presence of the antiferromagnetic SRO, i.e., spin excitations are suppressed, resulting in the deviation of the Curie-Weiss-like temperature dependence of $1/T_1T$ as well as giving rise to a broad peak around a cross-over temperature. In this

way, without assuming the real energy gap, we are still able to explain the observed gaplike temperature dependence. By hole doping, SRO will be rapidly suppressed, which will also be in accordance with the observed hole-concentration dependence of the spin-gap temperature T_s .

The Hamiltonian of the present study is the finite-size single-layer t - J model given by

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{j,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma}^\dagger c_{j,\sigma}) + J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j), \quad (1)$$

where t is the nearest-neighbor (NN) electron hopping integral and J is the antiferromagnetic Heisenberg exchange constant between spins on adjacent lattice sites. Throughout the paper, all the energies are measured in units of t . With the use of the calculated eigenvalues and eigenvectors, we evaluated the temperature dependence of the NMR relaxation rate $1/T_1$ by the following formula: [7]

$$\frac{1}{T_1 T} \propto \lim_{\omega \rightarrow 0} \frac{1}{\omega} \sum_q \text{Im} \chi(q, \omega), \quad (2)$$

where $\text{Im} \chi(q, \omega)$ is the imaginary part of the dynamical spin susceptibility of conduction electrons. The effect of the q -dependence of the hyperfine form factor is neglected, for simplicity. In actual numerical estimations of $\text{Im} \chi(q, \omega)$ the δ -function is approximated by the Lorentzian distribution with a small width $\epsilon = 0.01t$. In order to reveal the relation between the temperature dependence of the relaxation rate and SRO, the NN spin correlation function is also calculated by

$$C_1 = \frac{1}{N} \sum_i \frac{1}{4} \sum_{\rho=\pm\hat{x}, \pm\hat{y}} \langle S_i^z S_{i+\rho}^z \rangle. \quad (3)$$

Since we need all the eigenvalues and eigenvectors, the cluster size of the model was limited by the available disk space of the computer. We show, in Fig.1(a), the temperature dependence of $1/T_1T$ and NN spin correlation function for the $\sqrt{10} \times \sqrt{10}$ cluster with 0, 1 and 2 holes, corresponding to the hole concentrations, $\delta=0, 0.1$

and 0.2, respectively. We employ $J = 0.3$, estimated for cuprate superconductors. We clearly see a broad peak in the temperature dependence of $1/T_1T$ of the undoped system around the temperature $T \sim J$, which agrees with the temperature below which SRO begins to prevail.

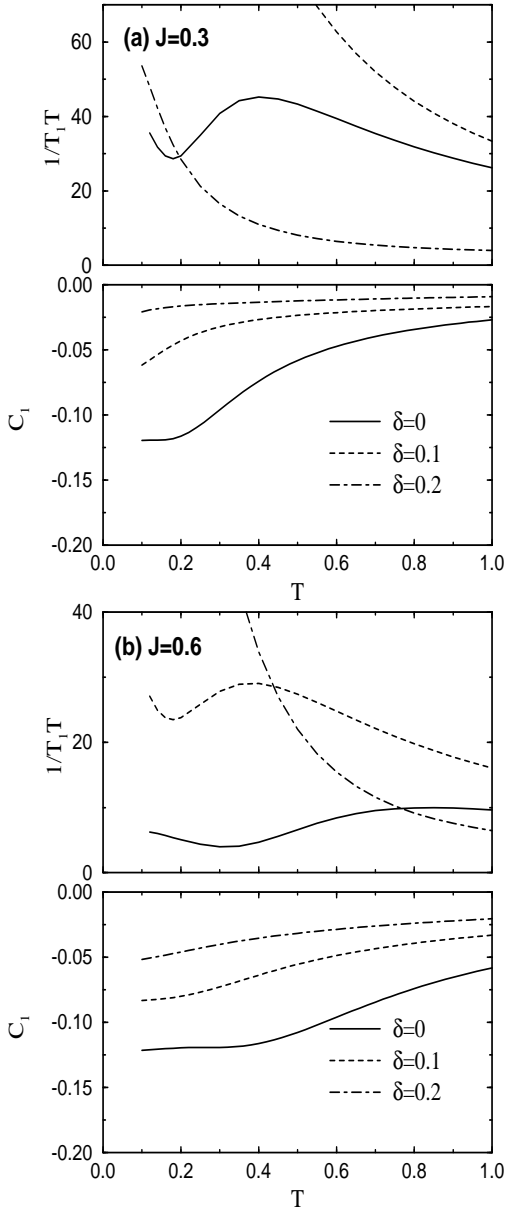


FIG. 1. Temperature dependence of $1/T_1T$ (the right hand side of (2) in the text) and NN spin correlation C_1 for (a) $J = 0.3$ and (b) $J = 0.6$.

Unfortunately no significant suppression of $1/T_1T$ is observed in systems with hole dopings, as shown in the same figure. This is, however, consistent with the absence of SRO in these systems. For small clusters, the relative importance of the effect of electron hopping tends to be overestimated for the fixed value of J . Therefore we also performed the same calculation assuming a larger param-

eter value of J ($=0.6$). From the T -dependence of $1/T_1T$ in Fig.1(b) with $\delta = 0.1$, we clearly see that the gaplike behavior is also present even in the doped system, which correlates well with the appearance of SRO. From the δ -dependence of the figure, we also see that the temperature region having SRO rapidly decreases with increasing hole concentration. Since the calculated lowest excitation gap of a $\sqrt{10} \times \sqrt{10}$ cluster with one hole is 0.146, the broad peak around $T \sim 0.4$ is not related to any finite size effects. We have confirmed that the same correlation between that $1/T_1T$ and SRO also exists on the $\sqrt{8} \times \sqrt{8}$ cluster with one hole ($\delta=0.125$), which suggests that the feature is a bulk property independent of the system size. The same calculation with hole dopings was reported for the 4×4 cluster [8] ($J/t = 0.3$). However, the temperature range did not cover the region where the peak of $1/T_1T$ was expected to be observed. We have confirmed that the broad peak structure in the T -dependence of $1/T_1T$ is almost independent of the Lorentzian width ϵ . The absolute values of $1/T_1T$, on the other hand, are very sensitive to our choice of ϵ in such small cluster calculations. Therefore the relative magnitude of the curves in Fig.1, evaluated by assuming the same ϵ value for several δ values, should not be taken seriously. For the same reason, $1/T_1T$ has a large but finite value at low temperature for $\delta = 0.2$.

In the Heisenberg model with no hole doping, the presence of the broad peak in the temperature dependence of $1/T_1T$ around $T \sim J$ has already been derived by Chakravarty and Orbach [9] based on the high-temperature series-expansion method. They also predicted that $1/T_1T$ shows a minimum in its T -dependence around $T \sim J/2$, which was later verified by the quantum Monte-Carlo calculation [10] for the case of local hyperfine coupling. The upturn behavior of $1/T_1T$ for $\delta = 0$ in our Figs.1(a) and 1(b) may arise by the above mechanism. Owing to the finite-size effects we must, however, be careful when drawing any definite conclusions concerning whether these minima will survive even in the presence of hole doping in the thermodynamic limit at low temperature. In bulk two-dimensional Heisenberg systems without hole doping, the broad peak at around $T \sim J$ may be difficult to observe as clearly as in Fig. 1, because the long-range antiferromagnetic order grows toward $T = 0$ at low temperature. A modified high-temperature series expansion study [11] actually yielded not such a clear peak, but a small shoulder in the temperature dependence of $1/T_1T$. Experimentally, though no peak structure in the T dependence of $1/T_1T$ for La_2CuO_4 has been observed by Imai *et al.*, [12] its absence is still controversial because the temperature range is limited to below $T \sim J$. On the other hand, in the case of systems with hole doping, we expect the peak behavior to be more easily observed than in the pure Heisenberg system, due to the absence of the antiferromagnetic long-range order in the ground state at $T = 0$ K.

In conclusion, we have succeeded in deriving the pseudogap behavior of high- T_c cuprates. We showed that a

broad peak appears in the temperature dependence of $1/T_1T$ because of the suppression of the dynamical susceptibility due to the development of SRO inherent to undoped low-dimensional Heisenberg antiferromagnets. It will be interesting to examine the effect of SRO on other dynamical quantities, such as neutron scattering intensities and the photoemission spectrum. We could also show that hole doping rapidly destroyed the SRO of the system, resulting in the observed hole-concentration dependence of the spin-gap temperature.

If the present scenario is true, the hole concentration dependence of the superconducting critical temperature T_c can be understood as follows. First the behavior seems to suggest that the antiferromagnetic SRO is necessary for the superconducting mechanism of high T_c cuprates to work. In the underdoped region, because the SRO is always present since $T_s > T_c$, T_c is mainly determined by some pairing mechanism, giving rise to the critical temperature proportional to the hole concentration. On the other hand, in the overdoped region, though the mechanism might indicate a higher T_c , it is upper-limited by T_s because of the disappearance of SRO. We are not concerned with the nature of the pairing mechanism of the superconductivity in the present paper. The presence of SRO, in this way, may play a significant role as a necessary condition for the occurrence of the high- T_c superconductivity.

We wish to thank Prof. Y. Hasegawa for fruitful discussions. We also thank the Supercomputer Center, Institute for Solid State Physics, University of Tokyo for the facilities and the use of the Fujitsu VPP500.

Phys. Rev. Lett. **70** (1993) 1002.

-
- [1] A. Goto, H. Yasuoka and Y. Ueda: J. Phys. Soc. Jpn. **65** (1996) 3043 and references therein.
 - [2] T. Tanamoto, K. Kuboki and H. Fukuyama: J. Phys. Soc. Jpn. **60** (1991) 3072.
 - [3] M. U. Ubens and P. A. Lee: Phys. Rev. **B50** (1994) 438.
 - [4] B. L. Altshuler, L. B. Ioffe and A. J. Millis: Phys. Rev. **B53** (1996) 415.
 - [5] Y. Itoh, T. Machi, A. Fukuoka, K. Tanabe and H. Yasuoka: J. Phys. Soc. Jpn. **65** (1996) 3751.
 - [6] K. Miyake and O. Narikiyo: J. Phys. Soc. Jpn. **63** (1994) 3821.
 - [7] T. Tohyama, H. Okuda and S. Maekawa: Physica **C215** (1993) 382.
 - [8] J. Jaklic and P. Prelovsek: Phys. Rev. Lett. **74** (1995) 3411.
 - [9] S. Chakravarty and R. Orbach: Phys. Rev. Lett. **64** (1990) 224.
 - [10] A. W. Sandvik and D. J. Scalapino: Phys. Rev. **B51** (1995) 9403.
 - [11] R. R. P. Singh and M. P. Gelfand: Phys. Rev. **B42** (1990) 996.
 - [12] T. Imai, C. P. Slichter, K. Yoshimura and K. Kosuge: